# A Manybody Formalism for Fermions, Enforcing the Pauli Principle on Paper

D.K. Watson

University of Oklahoma

Homer L. Dodge Department of Physics and Astronomy

Norman, OK 73019

(Dated: June 18, 2015)

Confined quantum systems involving $N$ identical interacting fermions are found in many areas of physics, including condensed matter, atomic, nuclear and chemical physics. In a previous series of papers, a manybody perturbation method that is applicable to both weakly and strongly-interacting systems of bosons has been set forth by the author and coworkers. A symmetry invariant perturbation theory was developed which uses group theory coupled with the dimension of space as the perturbation parameter to obtain an analytic correlated wave function through first order for a system under spherical confinement with a general two-body interaction. In the present paper, we extend this formalism to large systems of fermions, circumventing the numerical demands of applying the Pauli principle by enforcing the Pauli principle on paper. The method does not scale in complexity with $N$ and has minimal numerical cost. We apply the method to a unitary Fermi gas and compare to recent Monte Carlo values.

*Introduction.–* Confined quantum systems of fermions are widespread across physics. They include, for example, atoms, atomic nuclei, neutron stars, quantum dots, and cold Fermi gases. These systems possess from a few tens to millions of particles and span an enormous range of interparticle interaction strength presenting a challenge for $N$-body methods when mean-field approaches fail. In the last decade, ultracold Fermi gases have emerged as a testing ground for manybody methods due to their precise controllability in experiments. Using a magnetic field to tune the scattering length of atoms allows the exploration of the physics over many length scales, including the "unitary gas" defined by an infinite scattering length. Without a defining length scale other than the interparticle distance, the unitary gas does not yield to conventional perturbation treatments, typically requiring a full manybody treatment for an accurate description.

Fermi systems in the unitary regime are currently of great interest. This strongly interacting regime, stabilized by the Pauli exclusion principle, exists on the cusp of the BCS-BEC crossover and exhibits universal thermodynamic behavior which has been verified in the laboratory to within a few percent[1]. Verifying this universal behavior theoretically requires access to the partition function, i.e. the energy spectrum with degeneracies. Required resources on a classical computer for an *exact* solution of even the ground state of the $N$-body problem scale exponentially with $N$. Traditional full configuration interaction can cope with at most some ten particles[2] and methods such as coupled-cluster[3] with a computational time polynomial in $N$, $O(N^7)$, are extremely expensive. Quantum Monte Carlo (QMC) methods for fermions suffer from the so-called "sign" problem[4–6] resulting in an exponential growth in simulation times. Other methods that have been applied to strongly interacting Fermi systems include the method of correlated basis functions[7, 8], density functional theory[9], diagrammatic approaches[10], and the stochastic variational method [11, 12]. To date, the determination of the energy spectrum of systems containing four or more particles remains a challenge.[12]

In this paper, we investigate an alternative approach to study large systems of fermions. Our symmetry-invariant perturbation theory, SPT, offers a perturbation approach for a systematic study of correlation including the unitary regime. The perturbation parameter depends on the inverse dimensionality of space ($\delta = 1/D$), rather than the strength of the interaction, so SPT is equally applicable to weakly or strongly interacting systems. The method is essentially *analytic* [13], with $N$, the number of particles, entering as a parameter, allowing results for any $N$ to be obtained from a single calculation[14]. The lowest-order result includes correlation and in theory, can be systematically improved by going to higher order[15]. This method couples group theory with conventional dimensional perturbation theory (DPT)[16–18] to take advantage of the high degree of symmetry possible among identical particles in higher dimensions. The terms in the perturbation expansion are invariant under $N!$ symmetry operations, greatly reducing the number and complexity of the building blocks of these terms. This method currently includes full manybody effects that are exact through first order. Excited states are obtained from the same analytic calculation[14], differing only in the number of quanta in the different normal modes. In principle, the full energy spectrum is accessible.

In past work, DPT has been applied to fermion systems including single atoms[17, 19], quantum dots[20], and small molecules[21]. The symmetry invariant approach, SPT, has been applied thus far only to bosons with spherical confinement, determining first-order energies, normal mode frequencies[13, 14], the lowest-order SPT wave function[22] and density profile[23]. We ap-

plied these results to a BEC for which the density profile is a directly observable manifestation of the quantized behavior. In a later series of papers, we extended this work for bosons to first-order wave functions and density profiles[24, 25]. We demonstrated that this method effectively rearranges the numerical work for this manybody problem into analytic building blocks at each order giving the exact result order by order in the perturbation series[25, 26]. The complexity of the rearranged problem scales with the order of the perturbation series, not with the number of particles[26].

In this extension of SPT to fermions, we tackle the challenge of applying the Pauli principle, typically an expensive numerical task. We describe how this is achieved "on paper" for any value of $N$, thus circumventing heavy numerical effort. We apply the method in this initial study to large systems of cold fermions in the unitary regime for which a number of very accurate calculations are available. Results are obtained using analytic building blocks which have been calculated and stored previously and which have been extensively checked using an independent solution of a model system of harmonically confined, harmonically interacting particles[25]. Our results compare well to very accurate Monte Carlo results[8, 27] including some recent benchmark calculations using the auxilliary field Monte Carlo method[28].

We begin the perturbation analysis by defining dimensionally scaled quantities: $\bar{E} = \kappa(D)E$, and $\bar{H} = \kappa(D)H$ where $\kappa(D)$ is a scale factor which regularizes the large-dimension limit[22]. The scaled version of the Schrodinger equation becomes

$$\bar{H}\Phi = \left(\frac{1}{\kappa(D)}\bar{T} + \bar{V}_{\text{eff}}\right)\Phi = \bar{E}\Phi, \qquad (1)$$

where barred quantities indicate variables in scaled units $(\kappa(D) = D^2/(\hbar\bar{\omega}_{ho})$ for this work. See Ref. [22]). The term $\bar{T}$ contains the derivative terms of the kinetic energy and $\bar{V}_{\text{eff}}$ includes centrifugal, two particle, and confinement potentials[22].

We assume a totally symmetric, large-dimension configuration at which the effective potential is a minimum. The $N$ particles are arranged on a hypersphere, each particle with a radius, $\bar{r}_\infty$, from the center of the confining potential. Furthermore, the angle cosines between each pair of particles take on the same value, $\bar{\gamma}_\infty$, i.e.

$$\begin{aligned} \lim_{D\to\infty} \bar{r}_i &= \bar{r}_\infty \ (1 \le i \le N), \\ \lim_{D\to\infty} \gamma_{ij} &= \bar{\gamma}_\infty \ (1 \le i < j \le N). \end{aligned} \qquad (2)$$

(This symmetric high-dimensional structure is not unlike the localized structure found in a hyperspherical treatment of the confined two-component Fermi gas in the $N \to \infty$ limit[29].) In scaled units the $\delta \to 0$ $(D \to \infty)$ approximation for the energy is simply the effective potential minimum, i.e. $\bar{E}_\infty = \bar{V}_{\text{eff}}(\bar{r}_\infty, \bar{\gamma}_\infty; \ \delta = 0)$.

In this $\delta \to 0$ approximation, the centrifugal-like term that appears in $\bar{V}_{\text{eff}}$, which is nonzero even for the ground state, is a zero-point energy contribution satisfying the minimum uncertainty principle[30]. The value of $\bar{\gamma}_\infty$, which is zero in the *mean-field* approximation for the $L = 0$ angular momentum states considered here, is, in fact, *not* zero, an indication that beyond-mean-field effects are included in the $\delta \to 0$ limit.

This highly-symmetric, $\delta \to 0$ structure imparts a point group structure to the system which is isomorphic to the symmetric group of $N$ identical objects[31], $S_N$, allowing a largely analytic solution. The $\delta \to 0$ approximation may be systematically improved by using it as the starting point for a perturbation expansion[15]. The $S_N$ symmetry greatly simplifies this task since the interaction terms individually have to transform as a scalar under the $S_N$ point group.

The perturbation series has the form:

$$\begin{aligned} \bar{E} &= \bar{E}_\infty + \delta\sum_{j=0}^{\infty}\left(\delta^{\frac{1}{2}}\right)^j \bar{E}_j \\ \Phi &= \sum_{j=0}^{\infty}\left(\delta^{\frac{1}{2}}\right)^j \Phi_j. \end{aligned} \qquad (3)$$

In practice $\bar{E}_j = 0 \ \forall \ j$ odd. The $j = 0$ terms are obtained from a harmonic equation, and referred to as the energy and wave function at harmonic order. To obtain this harmonic correction for small values of $\delta$, we expand about the minimum of the $\delta \to 0$ effective potential.

The harmonic-order Hamiltonian is solved using the FG matrix method[32] to obtain the normal-mode frequencies, $\bar{\omega}_\mu$. The number of roots, $\lambda_\mu$, $(\lambda_\mu = \bar{\omega}_\mu^2)$, of the secular equation, $N(N + 1)/2$ roots, is potentially huge; however, due to the $S_N$ symmetry of the problem there is a reduction to five distinct roots,

The $\boldsymbol{FG}$ matrix is invariant under $S_N$, so it does not connect subspaces belonging to different irreducible representations (irreps.) of $S_N$[33]. Thus the normal coordinates must transform under irreps. of $S_N$. The normal coordinates are linear combinations of the elements of the internal displacement vectors which transform under reducible representations of $S_N$. One can show that these reduce to two 1-dimensional $[N]$ irreps. denoted by $\boldsymbol{0^+, 0^-}$, two $(N-1)$-dimensional $[N-1,1]$ irreps. denoted by $\boldsymbol{1^+, 1^-}$, and one angular $N(N-3)/2$-dimensional $[N-2,2]$ irrep. denoted by $\boldsymbol{2}$[13].

The energy through harmonic order in $\delta$ is [13]

$$\overline{E} = \overline{E}_\infty + \delta\left[\sum_{\substack{\mu=\{\boldsymbol{0^\pm, 1^\pm},\\ \boldsymbol{2}\}}}(n_\mu + \frac{1}{2}d_\mu)\bar{\omega}_\mu + v_o\right], \quad (4)$$

where $n_\mu$ is the total number of quanta in the normal mode with the frequency $\bar{\omega}_\mu$; $\mu$ is a label which runs over $\boldsymbol{0^-}$, $\boldsymbol{0^+}$, $\boldsymbol{1^-}$, $\boldsymbol{1^+}$, and $\boldsymbol{2}$, regardless of the number of particles in the system (see Refs. [13]and Ref.[15] in [22]), and $v_o$ is a constant. The multiplicities of the five roots are: $d_{\boldsymbol{0^+}} = 1$, $d_{\boldsymbol{0^-}} = 1$, $d_{\boldsymbol{1^+}} = N - 1$, $d_{\boldsymbol{1^-}} = N - 1$, $d_{\boldsymbol{2}} = N(N-3)/2$.

A character analysis of the normal modes reveals that the **2** normal modes are phonon, i.e. compressional modes; the $\mathbf{1}^{\pm}$ modes show single-particle character, and the $\mathbf{0}^{\pm}$ modes describe center-of-mass and breathing motions.

*Enforcing the Pauli Principle.–* To generalize SPT from quantum systems of bosons to quantum systems of fermions, we must enforce the Pauli principle, thus requiring the $N$-body wave function to be totally antisymmetric. This is enforced by placing certain restrictions on the occupancies of the normal modes, i.e. on the values of the normal mode quantum numbers, $n_\mu$, $\mu = \mathbf{0}^{\pm}, \mathbf{1}^{\pm}, \mathbf{2}$ in Eq. (4)[17]. The possible assignments can be found by relating the normal mode states $|n_{\mathbf{0}^+}, n_{\mathbf{0}^-}, n_{\mathbf{1}^+}, n_{\mathbf{1}^-}, n_{\mathbf{2}} >$ to the states of the confining potential which is a spherically symmetric three dimensional harmonic oscillator ($V_{\mathtt{conf}}(r_i) = \frac{1}{2} m \omega_{ho}^2 r_i{}^2$) for which the restrictions imposed by antisymmetry are known. These two series of states can be related in the double limit $D \to \infty$, $\omega_{ho} \to \infty$ where both representations are valid.

For large $D$, the normal mode description given by Eq. (4) is exact. Applying the large $\omega_{ho}$ limit results in:

$$E = N \frac{D}{2} \hbar \omega_{ho} + (2n_{\mathbf{0}^+} + 2n_{\mathbf{0}^-} + 2n_{\mathbf{1}^+} + 2n_{\mathbf{1}^-} + 2n_{\mathbf{2}}) \hbar \omega_{ho} \tag{5}$$

Now consider $\omega_{ho} \to \infty$ first and then $D \to \infty$. The harmonic oscillator levels are exact:

$$
\begin{aligned}
E &= \sum_{i=1}^{N} \left[ (2\nu_i + l_i) + \frac{D}{2} \right] \hbar \omega_{ho} \\
&= N \frac{D}{2} \hbar \omega_{ho} + \sum_{i=1}^{N} (2\nu_i + l_i) \hbar \omega_{ho}
\end{aligned}
\tag{6}
$$

where $\nu_i$ is a radial quantum number and $l_i$ the orbital angular momentum quantum number. Equating these two expressions which are equal in the double limit, the quantum numbers in the two representations can now be related to show the restrictions on normal mode states imposed by antisymmetry. Because of the clean separation of radial and angular motions, two conditions result:

$$
\begin{aligned}
2n_{\mathbf{0}^-} + 2n_{\mathbf{1}^-} &= \sum_{i=1}^{N} 2\nu_i \\
2n_{\mathbf{0}^+} + 2n_{\mathbf{1}^+} + 2n_{\mathbf{2}} &= \sum_{i=1}^{N} l_i
\end{aligned}
\tag{7}
$$

These equations determine a set of possible normal mode states $|n_{\mathbf{0}^+}, n_{\mathbf{0}^-}, n_{\mathbf{1}^+}, n_{\mathbf{1}^-}, n_{\mathbf{2}} >$ from the known set of permissible $L = 0$ harmonic oscillator configurations.

*Application: The Unitary Gas.–* The Schrödinger equation for an $N$-body system of fermions, $N = N_1 + N_2$ with $N_1$ spin up and $N_2$ spin down fermions, confined by
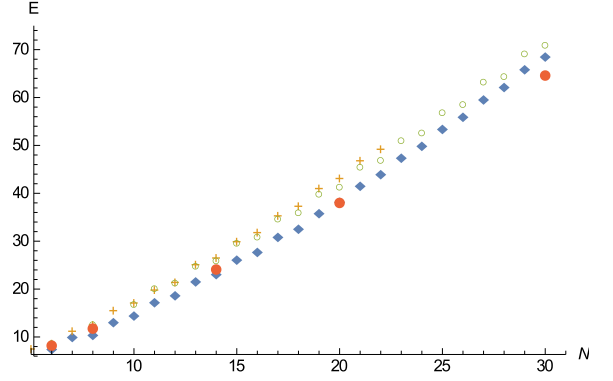


FIG. 1: Ground state energies of the harmonically trapped unitary Fermi gas (units $\hbar \omega_{ho} = 1$). Our first-order perturbation results (filled diamonds) are compared to GFMC (+'s)[27], fixed-node DMC (open circles) from Ref. [8], and AFMC results (filled circles, $N$=6, 8, 14, 20, 30 only)[28].

a spherically symmetric potential is

$$H\Psi = \left[ \sum_{i=1}^{N} h_i + \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} g_{ij} \right] \Psi = E\Psi . \tag{8}$$

where $h_i$ and $g_{ij}$ are the single-particle Hamiltonian and the two-body interaction potential, respectively. We assume a $T = 0K$ condensate with $N_1 = N_2$ confined by an isotropic, harmonic trap with frequency $\omega_{ho}$.

To study the unitary regime, we replace the actual atom-atom potential by an attractive square well potential of radius $R$:

$$V_{\mathtt{int}}(r_{ij}) = \left\{ \begin{array}{ll} -V_o , & r_{ij} < R \\ 0, & r_{ij} \geq R . \end{array} \right. , \tag{9}$$

For fixed range $R$, the potential depth $V_0$ is adjusted so the s-wave scattering length, $a_s$ is infinite. The range is selected so $R << a_{ho}$ ( $a_{ho} = \sqrt{\hbar/(m\omega_{ho})}$) and can be systematically reduced to extrapolate to zero-range interaction. We dimensionally continue the square well potential so that it is differentiable away from $D = 3$, allowing us to perform the dimensional perturbation analysis[13, 14]). Thus, we take the interaction to be

$$V_{\mathtt{int}}(r_{ij}) = V_0(\delta) \left[ 1 - \tanh\left[ \frac{1}{1-3\delta} \left( r_{ij} - 3\delta R \right) \right] \right] , \tag{10}$$

where $V_o(\delta) = \frac{1}{1-3b\delta}$. The potential depth $V_o$ is adjusted by adjusting the value of $b$ so the scattering length is infinite when $\delta = \frac{1}{3}$. This interaction becomes a square well of radius $R$ in the physical $D = 3$ limit. The functional form of the potential at $D \neq 3$ is not unique. Other forms could be chosen with equal success as long as the form is differentiable and reduces to a square well potential at $D = 3$. We simply choose a form that allows a gradual softening of the square well.

In Fig. 1 we plot the ground state energies from $N = 6$ to $N = 30$ and compare to Green's function
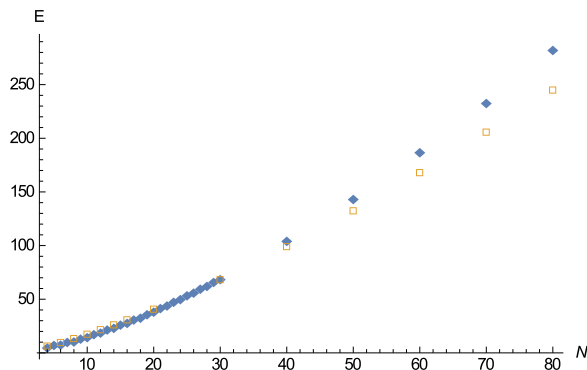
FIG. 2: Ground state energies of the harmonically trapped unitary Fermi gas (units $\hbar\omega_{ho} = 1$). Our first-order perturbation results (filled diamonds) are compared to DMC results Ref. [28] (open squares)

Monte Carlo (GFMC) energies[27], to fixed-node diffusion Monte Carlo (DMC) energies[8] which provide accurate upper bounds to the ground state energy, and to recent benchmark auxiliary field Monte Carlo calculations (AFMC)[28] which are exact, but subject to finite lattice size errors for which corrections have been made. The AFMC results are currently the most accurate results available. Our energies which include full many-body effects through first order compare well to these AFMC results and except for $N = 8$ they are slightly closer to the AFMC results than the GFMC and DMC results shown in Figure 1. Our numbers, as well as the GFMC and DMC numbers from Refs. [8, 27], show a distinct odd/even oscillation, but no obvious shell effects. Obtained from analytic building blocks that have been calculated and stored previously, our numerical requirements take a few seconds on a work station.

No parameters are used to obtain these results other than those used to produce a square well potential with infinite scattering length. For the GFMC and DMC stud-

ies shown in Figure 1, no results exist for values of $N$ higher than shown. Accurate results for higher $N$ are, of course, increasingly difficult to achieve. In Figure 2 we compare our results at first order above $N = 30$ with available DMC results from Ref. [28]. Our first-order results show the expected increase in error as N increases suggesting that for larger N, higher order terms may be necessary.

*Conclusions* – In this paper we have extended the symmetry-invariant perturbation method from bosons to fermions, applying the Pauli principle "on paper" to avoid heavy numerical expense. The method has been tested in the unitary regime, which is of particular interest for manybody methods since its infinite scattering length and the lack of a natural scale typically require intensive numerical simulation for an accurate description. Our analytic results through first order yield energies that are comparable in accuracy with recent Monte Carlo results. As $N$ increases, our error increases suggesting the need for higher order terms. It may also be possible to rearrange the perturbation series to minimize the importance of higher order terms.

The theory applied in this paper is applicable to $L = 0$ states of spherically confined systems with general attractive or repulsive interparticle interactions and is also applicable to both weakly and strongly correlated systems. The fact that $\overline{\gamma}_\infty$ is not zero is an indication that beyond-mean-field effects are included in this result even in the $D \to \infty$ limit. This theory is readily generalizable to systems with a cylindrical confining potential.

Higher-order calculations may be required for larger $N$. A detailed program for calculating higher-order DPT corrections to $N$-body systems has been laid out[15] and applied to high order for small-$N$ systems[34]. For large-$N$ systems the $S_N$ point-group symmetry greatly simplifies the calculation of these higher-order terms.

We thank Doerte Blume and Stefano Gandolfi for discussions and Monte Carlo results.

[1] H. Hu, P.D. Drummond, and X.-J. Liu, Nat. Phys. **3**, 469, (2007); M. Horikoshi et al. Science **327**, 442(2010); S. Nascimbene et al. Nature(London( **463**, 1057(2010); M.J.H. Ku et al., Science **335**, 563(2012); C. Cao et al., *ibid* **331**, 58(2011).

[2] G.H. Booth et al., Nature **493**. 365 (2013).

[3] See for example L.S. Cederbaum, O.E. Alon, and A.I. Streltsov, Phys. Rev. A **73**, 043609 (2006); R.J. Bartlett and M. Musial, Rev. Mod. Phys. **79**, 291 (2007).

[4] See for example D. Landau and K. Binder, *A Guide to Monte-Carlo Simulations in Statistical Physics*, (Cambridge University Press, Cambridge, 2001); M. Holzmann, W. Krauth, and M. Naraschewski, Phys. Rev. A **59**, 2956 (1999).

[5] K.E. Schmidt and M.H. Kalos, in K. Binder(ed.): *Applications of the Monte Carlo Method in Statisitcal Physics* (Springer, 1984).

[6] M. M. Forbes, S. Gandolfi and A. Gezerlis, Phys. Rev. A

**86**, 053603 (2012).

[7] See for example S. Fantoni and A. Fabrocini, in it Microscopic Quantum Many Body Theories and Their Applications, J. Navarro and A. Polls eds., Lecture Notes in Physics Vol. 150 (Springer-Verlag, Berlin, 1998) p. 119.

[8] D. Blume, J. von Stecher, and C. H. Greene, Phys. Rev. Lett. **99**, 233201(2007).

[9] W. Kohn, Rev. Mod. Phys. **71**, 1253 (1999).

[10] H. Hu, X.-J. Liu, and P.D. Drummond, Europhys. Lett. **74**, 574(2006).

[11] K. Varga, Y. Suzuki, Phys. Rev. C. **52**, 2885(1995).

[12] K.M. Daily and D. Blume, Phys. Rev. A **81**, 053615 (2010).

[13] B.A. McKinney et al., Ann. Phys. (NY) **310**, 56 (2003).

[14] B.A. McKinney, M. Dunn, D.K. Watson, Phys. Rev. A **69**, 053611 (2004).

[15] M. Dunn et al., J. Chem. Phys. **101** 5987 (1994).

[16] *Dimensional Scaling in Chemical Physics*, edited by D.R.

Herschbach, J. Avery, and O. Goscinski (Kluwer, Dordrecht, 1992).

[17] J.G. Loeser, J. Chem. Phys. **86**, 5635 (1987).

[18] A. Chatterjee, Phys. Rep. **186**, 249 (1990).

[19] L.D. Mlodinow and N. Papanicolaou, Ann. Phys.(N.Y.) **131** 1 (1981); J.M. Rost, J. Phys. Chem. **97** 2461 (1993); G.F. Kventsel and J. Katriel, Phys. Rev. A **24**,2299 (1981).

[20] B.A. McKinney and D.K. Watson, Phys. Rev. B **61**, 4958 (2000).

[21] S.-W. Huang et al., Phys. Rev. A **58**, 250 (1998); A. A. Svidzinsky, M. O. Scully, and D. R. Herschbach, Phys. Rev. Lett. **95**, 080401, 2005.

[22] M. Dunn, D.K. Watson, and J.G. Loeser, Ann. Phys. (NY), **321**, 1939 (2006).

[23] W.B. Laing, M. Dunn, and D.K. Watson, Phys. Rev. A **74**, 063605 (2006).

[24] W.B. Laing, M. Dunn, and D.K. Watson, J. of Math. Phys. **50**, 062105 (2009).

[25] W.B. Laing et al., J Phys A **42**, 205307 (2009); M. Dunn et al., Phys. Rev A **80**, 062108 (2009).

[26] D.K. Watson and M. Dunn, Phys. Rev. Lett. **105**, 020402 (2010).

[27] S.Y. Chang and G.F. Bertsch, Phys. Rev. A **76**, 021603 (2007).

[28] J. Carlson and S. Gandolfi, Phys. Rev. A **90** 011601(R) (2014).

[29] S. T. Rittenhouse, et al., arXiv:cond-mat/0510454.

[30] A. Chatterjee, J. Phys. A: Math. Gen. **18**, 735 (1985).

[31] See for example M. Hamermesh, *Group Theory and its Application to Physical Problems*, (Addison-Wesley, Reading, MA, 1962).

[32] E.B. Wilson, Jr., J.C. Decius, P.C. Cross, *Molecular vibrations: The theory of infrared and raman vibrational spectra*. McGraw- Hill, New York, 1955.

[33] See for example reference 32, Appendix XII, p. 347.

[34] J.R. Walkup et al., Phys. Rev. A, **58**, 4668, (1998); J.C. Carzoli, M. Dunn and D.K. Watson, Phys. Rev. A **59**, 182 (1999); J.R. Walkup, M. Dunn, and D.K. Watson, J. Math. Phys. **41**, 218 (2000); J.R. Walkup, M. Dunn, and D.K. Watson, Phys. Rev. A **63**, 025405 (2001).